Ethyl hexanoate

123-66-0 | DTXSID3021980

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -76.4 °C

Global applicability domain: Inside

Local applicability domain index: 9.93e-01

Confidence level: 8.17e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl hexanoate
Measured: -67.0
Predicted: -76.4

Image not found
Hexyl acetate
Measured: -80.9
Predicted: -69.9

Image not found
Pentyl propionate
Measured: -73.1
Predicted: -76.6

Image not found
Propyl valerate
Measured: -70.7
Predicted: -76.7

Image not found
Butyl butyrate
Measured: -91.5
Predicted: -76.8